Activating Oxygen Chemistry for Sustainable Energy

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The development of sustainable energy is one of the most important scientific challenges in the 21st century. A critical element for sustainable energy implementation is to have efficient energy conversion and storage. Activating oxygen chemistry/electrochemistry is central to enable efficient oxidation of small molecules of energy consequence, photoelectrochemical and electrolytic water-splitting, fuel cells, and metal-air batteries. Probing a fundamental catalyst “design” principle” that links surface structure and chemistry to the catalytic activity can guide the search for highly active catalysts that are cost effective and abundant in nature. While such a design concept exists for metal catalysts, little is known about the design principles for activating oxygen redox on oxides. Recent advances in identifying the design principles and activity descriptors of transition metal oxides will be presented. We will show that these fundamental concepts can be used to tune transition metal oxide surfaces with much enhanced catalytic activities. Moreover, we will discuss how oxide bulk electronic structures can influence the catalytic activities of oxides, from which two different reaction mechanisms are proposed. Lastly, connecting bulk to surface electronic structures is challenging but much needed to provide mechanistic insights, and some in-situ synchrotron X-ray measurements to this end will be discussed.